Jornada Científica de la Sociedad Española de Arcillas

Madrid, 17 de noviembre de 2023

ICMM-CSIC y UAM

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Junta Directiva de la Sociedad Española de Arcillas

Programa de la Jornada:

11:00-11:30h Entrega de documentación y café

11:30-11:45h Acto de apertura en el Salón de Actos del ICMM-CSIC

11:45-12:45h Conferencia invitada impartida por el Presidente anterior de la SEA, Prof. Dr. Fernando Nieto García: “TEM y arcillas. La historia continúa”

13:00-14:45h Comida en El Goloso Campus

15:00-16:00h Sesión de posters

16:00-17:00h Asamblea de la Sociedad

17:00-17:15h Entrega de Premio a Jóvenes Investigadores por mejor Póster de Investigación y Ceremonia de Clausura

Listado de Conferencias y Trabajos Científicos:

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	Conferencia Invitada: TEM Y ARCILLAS. LA HISTORIA CONTINÚA. Fernando Nieto García
1	ANÁLISIS DEL FACTOR TEXTURAL EN LA DISTRIBUCIÓN DE ELEMENTOS POTENCIALMENTE TÓXICOS EN RESIDUOS MINERALÚRGICOS: GRUPO MINERO DE SAN QUINTIN (CIUDAD REAL) Alcorta, S., Crespo-Feo, E., Esbrí, J. M.
2	GENERATION AT RELATIVELY LOW TEMPERATURES OF GRAPHENE-LIKE MATERIALS SUPPORTED ON SEPIOLITE Barra, A., Ruiz-García, C., Lazăr, O., Mihai, G., Bratu, C., Darder, M., Aranda, P., Enăchescu, M., Nunes, C., Ferreira, P., Ruiz-Hitzky, E.
3	SÍNTESIS DE NANOARQUITECTURAS MOF/ARCILLA Y SU PROCESADO PARA APLICACIONES DE REMEDIACIÓN AMBIENTAL Boizas-González, L., Pérez-Carvajal, J., Aranda, P.
4	EXPANSION AND SEDIMENTATION BEHAVIOR OF COMPACTED BENTONITES IN ARTIFICIAL SMOOTH FRACTURES Dieguez, M., Morejon, J., Mingarro, M., García-Gutiérrez, M., Missana, T., Sellin, P., Alonso, U.
5	DISORDER IN KAOLINITE: XRD-IR SYSTEMATICS García-Vicente, A., Siranidi, E., García-Romero , E., Suárez, M., Chryssikos, G.D.
6	HINCHAMIENTO DE DOS BENTONITAS A ALTAS TEMPERATURAS Gimeno, N., Iglesias, R.J., Villar, M.V.
7	APLICACIÓN DE ÓXIDOS MIXTOS DE CaAlFe EN LA CAPTURA DE CO_2 PREPARADOS VÍA HIDROCALUMITA A PARTIR DE ESCORIA SALINA DE ALUMINIO Jiménez, A., Trujillano, R., Rives, V., Soria, M., Madeira, L.M., Vicente M.A.
8	EL CONTROL DE LOS MINERALES DE LA ARCILLA EN LA DISTRIBUCIÓN DE METALES CRÍTICOS EN PROCESOS DE METEORIZACIÓN QUÍMICA Laita, E., Bauluz, B., Yuste, A., Mayayo, M.J.
9	SÍNTESIS Y CARACTERIZACIÓN DE ESMECTITAS RICAS EN HIERRO Fe(II) Y Fe(III) PARA EL ESTUDIO DE PROCESOS REDOX EN EL MARCO DE UN AGP León, F.J., Fernández, A.M., Missana, T., Nieto, P.
10	VARIABILIDAD CRISTALOQUÍMICA Y FÓRMULAS ESTRUCTURALES DE ESMECTITAS DIOCTAÉDRICAS Lorenzo, A., García-Romero, E., Suárez, M.
11	CARACTERIZACIÓN DE MINERALES SECUNDARIOS FLUORURADOS ADSORBIDOS EN LA SUPERFICIE DE CENIZA VOLCÁNICA (TAJOGAITE, ESPAÑA): POSIBILIDAD DE REMEDIACIÓN DE ELEMENTOS POTENCIALMENTE TÓXICOS CON ZEOLITAS Martínez-del-Pozo, I., Arroyo, X., Esbrí J. M., López-Andrés, S.
12	EXPLORACIÓN DE LA INCORPORACIÓN DE ANFOTERICINA B EN ARCILLAS E HIDRÓXIDOS LAMINARES Misol, A., Martínez-Pacheco, A., Darder, M., Aranda, P.
13	SÍNTESIS DE ÁRIDOS LIGEROS ZEOLITIZADOS A PARTIR DE CAOLÍN Y RESIDUOS DE CAUCHO Moreno-Maroto, J.M., Rodríguez-Ortega, A.M., Cuevas, J., Regadío, M., Alonso-Azcárate, J.
14	DISEÑO EXPERIMENTAL PARA LA EVALUACIÓN DE BIOBARRERAS APLICADAS A VERTEDEROS Morita, A. K.M., Cuevas, J., Regadio, M.
15	EFECTOS DE LA ADICIÓN DE $FeCl_2$ EN BENTONITAS SOMETIDAS A UN GRADIENTE HIDROTERMAL Mota-Heredia, C., Cuevas, J., Fernández, R.
16	EVOLUCIÓN QUÍMICA DEL AGUA INTERSTICIAL EN LAS UNIDADES INFERIORES DE LA FORMACIÓN OPALINUS CLAY EN EL LABORATORIO SUBTERRÁNEO DE MONT TERRI (SUIZA) Nieto, P., Fernández, A.M., León, F.J.

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17	MINERALES DE LA ARCILLA EN PERFILES EDÁFICOS DE LA PENÍNSULA BYERS (ISLA LIVIGSTON, ANTÁRTIDA) Pelayo, M., Schmid, T., Saldaña, R., López-Martínez, J.
18	MINERALOGÍA DE ARCILLAS DE SUELOS DE LA SIERRA DEL ARAMO (ASTURIAS) Ramírez, J.D., Santamaría, A., Morales, J., García-Romero, E., Suárez, M.
19	HIDRÓXIDOS DOBLES LAMINARES EN LA CONVERSIÓN DE PLÁSTICOS A HIDRÓGENO Ruiz-Garcia, C., Baeza, J.A., Calvo, L., Prevot, V., Forano, C., Gilarranz, M.A.
20	EFECTO DE LA IRRADIACIÓN-GAMMA EN LAS PROPIEDADES SUPERFICIALES DE LA ARCILLA BENTONITA Soto-Ruiz, C., Alonso, U., Missana, T.
21	LÍMITES DE DETECCIÓN DE MINERALES ARCILLOSOS EN PRESENCIA DE CARBONATOS MEDIANTE ESPECTROSCOPÍA VNIR-SWIR Santamaría-López, Á., Suárez, M., García-Romero, E.
22	AMMONIUM CONCENTRATION IN STREAM SEDIMENTS RESULTING FROM DECADES OF DISCHARGE FROM A WASTEWATER TREATMENT PLANT Tijero, M., Valdepeñas, L., Gonzalez, J., Cuevas, J.
23	FILOSILICATOS PORTADORES DE LITIO EN TOBAS LITÍFERAS DEL CAMPO VOLCÁNICO DE MACUSANI, PUNO, PERÚ Villanova-de-Benavent, C., Segovia-More, M., Torró, L., Cuevas, J., Ruiz, A.I., Proenza, J.A., Nieto, F.
24	EFECTO DEL GRADIENTE TÉRMICO EN LA CONCENTRACIÓN DE SALES SOLUBLES DE UNA BENTONITA SÓDICA Zabala, A.B., Villar, M.V., Melón, A.M., Cuevas, J.

DISORDER IN KAOLINITE: XRD-IR SYSTEMATICS

GARCÍA-VICENTE, A.[1*], SIRANIDI, E.[2], GARCÍA-ROMERO, E.[3,4], SUÁREZ, M.[1], CHRYSSIKOS, G.D.[2]

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Kaolinite is a 1:1 dioctahedral phyllosilicate characterized by the stacking of 1:1 layers, which are held together by hydrogen bonds. Several authors have proposed models of stacking disorder based on the XRD patterns of kaolinite, such as layer distortions, a pseudo-mirror plane passing through the octahedral B-vacancy site, or alternating t_1 and t_2 layer displacements as the main possible stacking faults (Plançon et al., 1989).

Recent efforts have been conducted to correlate the kaolinite disorder parameters derived from X-ray measurements with infrared spectroscopic features (Drits et al., 2021; Pineau et al., 2022). These studies aimed at providing higher throughput methods for evaluating stacking disorder by elucidating how the latter affects the vibrational modes of kaolinite. XRD-infrared correlations often involved tedious deconvolution procedures or the recording of very subtle changes in the second and third derivative spectra. The objective of the present work was to revisit this issue on the basis of a new set of kaolinite samples spanning a broad range of disorder. In addition to testing correlations based on individual infrared proxies (positions, widths and relative intensities of infrared bands), PLS chemometric methodologies were also developed (Gionis et al., 2007).

For this purpose, 20 kaolinite natural samples in random powder form have been evaluated by X-ray diffraction (XRD), attenuated total reflectance (ATR) in the mid-infrared and diffuse reflectance Fourier Transform near-infrared (FT-NIR). X-ray diffraction patterns were collected using a X'Pert PRO MPD PANanalytical diffractometer with theta-2theta configuration in molybdenum radiation (Mo $K_{\alpha 1.2}$, λ=0.709 Å). The degree of structural disorder of kaolinite was evaluated using the Liétard (R2) index, the Hinckley index (HI) and AGFI index on the basis of XRD patterns in the 8-11°2θ and 15-19°2θ range. The ATR spectra of kaolinite (4000-600 cm^{-1}, 2 cm^{-1} resolution, 200 scans) were measured on a Fourier transform spectrometer (Tensor 2 by Bruker) equipped with a single reflection diamond ATR accessory (Miracle by Pike Technologies). The FT-NIR spectra were measured with a Fourier Transform spectrometer (Vector 22N by Bruker) in the range between 4000-8000 cm^{-1} with a resolution of 4 cm^{-1} (200 scans).

Several models of correlation were tested and compared. An example of the PLS multivariate modelling of the Liétard index (R2) is shown in Figure 1. This PLS prediction algorithm was cross-validated by the leave-one-out method on the basis of the FT-NIR spectra of the 20 kaolinites. The spectra over the 8000-4000 cm^{-1} wavenumbers range were vector-normalized

in the 1st derivative mode (Savitzky-Golay, 9pt smoothing, $\Delta\nu$ = 2 cm^{-1}). The model was optimized at three ranks leading to R^2 = 0.91 and a RMS error of cross validation better than 0.1. As such, it compares favourably to the current state-of-the-art and could facilitate the fast and non-invasive prediction of kaolinite disorder based on NIR spectral acquisition.

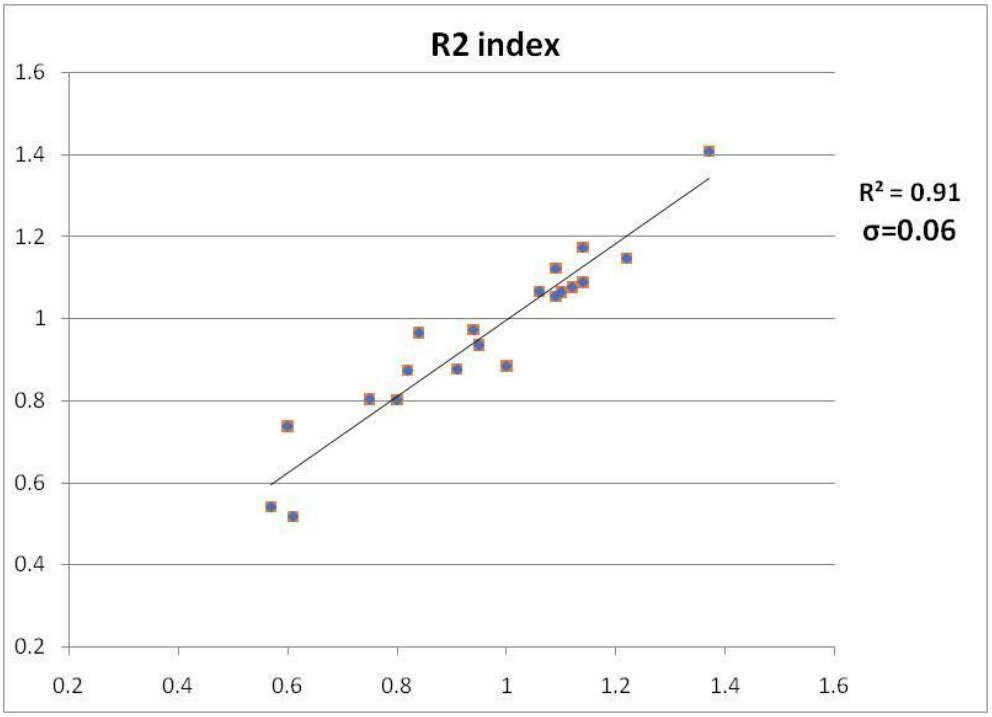

Figure 1: PLS multivariate prediction of Liétard index (R2) and FT-NIR spectra.

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